

## JUAN YANG

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### HIGHLIGHTS

- Expertise in molecular spectroscopy, optics, electronics, applications of lasers, and other aspects of physical and analytical chemistry.
- Five years of research experience using a Coherent Innova 20 argon ion laser and an ISA JY U-1000 spectrometer to collect high-temperature vapor-phase Raman spectra.
- Five years of research experience operating a Bomem DA8.02 Fourier-transform spectrometer to collect IR, Vis, and UV spectra.
- Three years of research experience in optical alignments and operation with a Nd:YAG pumped OPO laser for collecting supersonic jet-cooled LIF spectra.
- Experience in using a Verdi V-10 argon ion laser and a Quanta-Ray PDL-2 pulsed dye laser system.
- Expertise in high vacuum techniques.
- Computer programming in LabVIEW, C, and FORTRAN77.
- Expertise with electronic structure calculations using DFT and *ab initio* methods such as HF, MP2 for ground and CIS for excited electronic states to calculate energy, optimized structure, vibrational frequencies, etc.
- Excellent teamwork ability.

### EDUCATION

**Ph.D. / Chemistry** Overall GPA: 3.85/4.00 Degree Plan GPA: 4.00/4.00

Texas A&M University, College Station, TX, May 2006

Dissertation: Spectroscopic Investigations of the Vibrational Potential Energy Surfaces in Electronic Ground and Excited States (Prof. Jaan Laane)

**B.S. / Chemistry** GPA: 3.75/4.00

Beijing University (Peking University), Beijing, P. R. China, 2001

### EXPERIENCE

2001-Present **Department of Chemistry, Texas A&M University**, College Station, TX

Postdoctoral Research Associate. Research focused on attaining a detailed understanding of electronic excited state through which all photochemical processes occur. Utilized supersonic jet-cooled laser induced fluorescence (LIF) spectroscopy, including both fluorescence excitation (FES) and single vibronic level fluorescence (SVLF) spectroscopies, to determine the vibrational potential energy surfaces which govern the conformational and structural changes in the ground and excited electronic states of certain organic molecules.

Graduate Research Assistant. Investigated the vibrational potential energy surfaces and structures in the ground and excited electronic states of cyclic and bicyclic molecules including tetralin, 1,4-benzodioxan, coumaran, cyclopropanone, 1,3-dithiolane, and 3,7-dioxabicyclo[3.3.0]oct-1,5-ene. Spectroscopic methods such as FTIR, high temperature laser Raman, UV, and supersonic jet-cooled fluorescence spectroscopies were utilized. Theoretic calculations using HF, MP2, DFT, CIS methods were carried out to predict energy, structure, and vibrational frequencies in both ground and excited electronic states.

Graduate Teaching Assistant. Taught undergraduate general chemistry laboratories and graded for advanced physical chemistry.

2000-2001 **Department of Applied Chemistry, Beijing University**, Beijing, China

Undergraduate Research Assistant. Extraction and purification of saponins from panax notoginseng, a Chinese medicine that is a superb blood tonic and blood cleanser.

## PUBLICATIONS

- “Fluorescence, Ultraviolet Absorption Spectra, and the Structure and Vibrations of 1,2,3,4-Tetrahydronaphthalene in Its  $S_1(\pi,\pi^*)$  State.” **J. Yang**, M. Wagner, and J. Laane. (To be submitted to J. Chem. Phys.).
- “Laser Induced Fluorescence and Ultraviolet Absorption Spectra and the Ring-Puckering Potential Function of 1,4-Dihydronaphthalene in Its Ground and  $S_1(\pi,\pi^*)$  Electronic States.” M. Z. M. Rishard, M. Wagner, **J. Yang**, and J. Laane, J. Chem. Phys. Lett. (Submitted).
- “Theoretical Calculations and Vibrational Spectra of 1,4-Benzodioxan in Its  $S_1(\pi,\pi^*)$  Electronic Excited State.” **J. Yang**, J. Choo, O. Kwon, and J. Laane, Spectrochim. Acta Part A. (In press).
- “Spectroscopic Determination of Vibrational Potential Energy Surfaces in Ground and Excited Electronic States.” J. Laane and **J. Yang**, J. Electron Spectrosc. Relat. Phenom. (In press).
- “Calculation of Kinetic Energy Functions for the Ring-Twisting and Ring-Bending Vibrations of Tetralin and Related Molecules.” **J. Yang** and J. Laane, J. Mol. Struct., **798(1-3)**, 27 (2006).
- “Fluorescence and Ultraviolet Absorption Spectra and Structure of Coumaran and Its Ring-Puckering Potential Energy Function in the  $S_1(\pi,\pi^*)$  Excited State.” **J. Yang**, M. Wagner, K. Okuyama, K. Morris, Z. Arp, J. Choo, N. Meinander, O. Kwon, and J. Laane, J. Chem. Phys., **125**, 034308 (2006).
- “Laser-Induced Fluorescence Spectra, Structure, and the Ring-Twisting and Ring-Bending Vibrations of 1,4-Benzodioxan in Its  $S_0$  and  $S_1(\pi,\pi^*)$  States.” **J. Yang**, M. Wagner, and J. Laane, J. Phys. Chem. A, **110**, 9805 (2006).
- “The  $S_0$  Ring-Puckering Potential Energy Function for Coumaran.” **J. Yang**, K. Okuyama, K. Morris, and J. Laane, J. Phys. Chem. A, **109**, 8290 (2005).
- “Synthesis, Raman Spectrum, *Ab Initio* Calculations, and Structure of 3,7-Dioxabicyclo [3.3.0]oct-1,5-ene.” C. Mlynek, H. Hopf, **J. Yang**, and J. Laane, J. Mol. Struct., **742**, 161 (2005).
- “High-Temperature Vapor-Phase Raman Spectra of Non-Rigid Molecules.” J. Laane, **J. Yang**, D. Autrey, Z. Arp, K. Haller, M. Rishard, K. McCann, A. Combs, A. Jensen, and D. Meyer, Proc. Int. Conf. Raman Spectroscopy, **19**, 188 (2004).
- “Vibrational Frequencies and Structure of Cyclopropenone from *Ab Initio* Calculations.” **J. Yang**, K. McCann, and J. Laane, J. Mol. Struct., **695-696**, 339 (2004).
- “Vibrational Spectra and DFT Calculations of Tetralin and 1,4-Benzodioxan.” D. Autrey, **J. Yang**, and J. Laane, J. Mol. Struct., **661-662**, 23 (2003).

## PRESENTATIONS

- Industry-University Cooperative Chemistry Program (IUCCP), October 2006, College Station, Texas. “Vibrational Spectra, Structure, and the Ring-Puckering Potential Energy Functions in the  $S_0$  and  $S_1(\pi,\pi^*)$  Electronic States of Coumaran.”
- Texas Section of the APS Joint Fall Meeting, October 2006, Arlington, Texas. “Vibrational Spectra and Structure of Coumaran and Its Ring-Puckering Potential Energy Functions in the  $S_0$  and  $S_1(\pi,\pi^*)$  Electronic States.”

- International Conference on Raman Spectroscopy, August 2006, Yokohama, Japan. "Raman Spectra, Computations, and Structure of 2-Indanol, 2-Cyclohexenone, Dipicolinic Acid, 1,3-Dithiolane, and Pyrindan."
- International Conference on Electronic Spectroscopy and Structure, August 2006, Foz do Iguacu, Brazil. "Spectroscopic Determination of Vibrational Potential Energy Surfaces in Ground and Excited Electronic States."
- 21<sup>st</sup> Austin Symposium on Molecular Structure, March 2006, Austin, Texas. "Spectroscopic Determination of Molecular Structures and Potential Energy Surfaces of Cyclic and Bicyclic Molecules in their Ground and Excited Electronic States."
- 21<sup>st</sup> Austin Symposium on Molecular Structure, March 2006, Austin, Texas. "Spectra and DFT Calculations for the Vibrations of Tetralin and 1,4-Benzodioxan."
- 60<sup>th</sup> Ohio State International Symposium on Molecular Spectroscopy, June 2005, Columbus, Ohio. "Vibrational, Electronic, and Fluorescence Spectra and *Ab Initio* Calculations of 1,4-Benzodioxan."
- APS Regional Meeting, March 2005, Nacogdoches, Texas. "Fluorescence and Absorption Spectra and Potential Energy Surfaces of 1,3-Benzodioxole and Coumaran in their  $S_0$  and  $S_1(\pi, \pi^*)$  States."
- APS Regional Meeting, March 2005, Nacogdoches, Texas. "Infrared, Raman, Ultraviolet Absorption, Fluorescence Excitation and Single Vibronic Level Fluorescence Spectra and *Ab Initio* Calculations of 1,4-Benzodioxan."
- XXVII European Congress on Molecular Spectroscopy, September 2004, Krakow, Poland. "Ultraviolet Fluorescence and Cavity Ringdown Absorption Spectra and Structures of Enones and Aromatic Bicyclic Molecules in Their Singlet and Triplet Excited States."
- International Conference on Raman Spectroscopy, August 2004, Brisbane, Australia. "High-Temperature Vapor-Phase Raman Spectra of Non-Rigid Molecules."
- 20<sup>th</sup> Austin Symposium on Molecular Structure, March 2004, Austin, Texas. "Vibrational Frequencies and Structure of Cyclopropanone from *Ab Initio* Calculations."
- 20<sup>th</sup> Austin Symposium on Molecular Structure, March 2004, Austin, Texas. "Spectroscopic Determination of Vibrational Potential Energy Surfaces of Molecules in their Electronic Excited Singlet and Triplet States."

## REFERENCES

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